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ARL-TR-5088 **February 2010**

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REPORT DOCUMENTATION PAGE	Form Approved OMB No. 0704-0188

1. REPORT DATE *(DD-MM-YYYY)*	2. REPORT TYPE	3. DATES COVERED (From - To)
February 2010	Final	October 2005–October 2009

4. TITLE AND SUBTITLE
A Detailed, Finite-Rate, Chemical Kinetics Mechanism for Monomethylhydrazine-Red Fuming Nitric Acid Systems

5a. CONTRACT NUMBER

5b. GRANT NUMBER

5c. PROGRAM ELEMENT NUMBER

6. AUTHOR(S)
William A. Anderson, Michael J. McQuaid, Michael J. Nusca, and Anthony J. Kotlar

5d. PROJECT NUMBER
611102-AH43

5e. TASK NUMBER

5f. WORK UNIT NUMBER

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)
U.S. Army Research Laboratory
ATTN: RDRL-WML-D
Aberdeen Proving Ground, MD 21005-5066

8. PERFORMING ORGANIZATION REPORT NUMBER
ARL-TR-5088

9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)

10. SPONSOR/MONITOR'S ACRONYM(S)

11. SPONSOR/MONITOR'S REPORT NUMBER(S)

12. DISTRIBUTION/AVAILABILITY STATEMENT
Approved for public release; distribution is unlimited.

13. SUPPLEMENTARY NOTES

14. ABSTRACT
Between 2003 and 2005, a detailed, multistep, finite-rate chemical kinetics mechanism was developed to provide a basis for modeling monomethylhydrazine-red fuming nitric acid (MMH-RFNA) ignition and combustion chemistry. It was assembled almost entirely from reaction rate expressions and thermochemical data developed and validated for other combustion systems. When the mechanism's development was discontinued in 2005, it was composed of rate expressions for 513 reactions and involved 81 species. A lack of relevant experimental data limited the extent to which it could be validated as a whole. Nevertheless, when a subset of the mechanism was employed as a submodel for a computational fluid dynamics (CFD) model of an impinging stream vortex engine (ISVE) fueled with MMH-RFNA, the CFD model produced simulations whose calculations for chamber pressure and thrust well-reproduced ISVE test firing data. As such, the mechanism is considered to have a reasonable measure of validity and, thus, to be a good starting point for obtaining more refined MMH-RFNA mechanisms. This report discusses the mechanism's development and provides the rate expressions and thermochemical data that compose it. The sources of the rate expressions and thermochemical data are also provided.

15. SUBJECT TERMS
hypergolic combustion, kinetic mechanism, monomethylhydrazine, IRFNA

16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT	18. NUMBER OF PAGES	19a. NAME OF RESPONSIBLE PERSON
a. REPORT	b. ABSTRACT	c. THIS PAGE			William R. Andersen
Unclassified	Unclassified	Unclassified	UU	36	19b. TELEPHONE NUMBER (*Include area code*) 410-306-0731

Standard Form 298 (Rev. 8/98)
Prescribed by ANSI Std. Z39.18

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1. Introduction

This report discusses a detailed, finite-rate, chemical kinetics mechanism that was developed to provide a basis for modeling the ignition and combustion chemistry of systems fueled with monomethylhydrazine (MMH) and red fuming nitric acid (RFNA). Pursued between 2003 and 2005, the effort to develop a mechanism for this hypergolic (bipropellant) combination arose in conjunction with an effort to develop a computational fluid dynamics (CFD) model capable of simulating the combustion chamber dynamics of the U.S. Army Aviation and Missile Research, Development, and Engineering Center's (AMRDEC's) impinging stream vortex engine (ISVE). Conceived in the 1960s, but not developed in earnest until the 1990s, the first ISVEs built and tested by AMRDEC were fueled with MMH and inhibited RFNA (IRFNA) (Michaels and Wilson, 1995). Although hypergolic rocket motors that employ MMH and IRFNA in combination with one another do not appear to ever have been fielded, MMH and IRFNA are standard rocket propellants that, both individually and when mixed, have properties that make MMH-IRFNA a natural candidate for tactical missile applications. And AMRDEC was able to fly an ISVE fueled with the pair, confirming its utility for the application.

The CFD model ARL developed to simulate the ISVE's combustion chamber dynamics was derived from the ARL-NSRG3 code (Nusca, 2002). Of the many issues addressed in developing the code for modeling such systems, one was the specification of a representation of the reaction kinetics underlying MMH-IRFNA's ignition and combustion. As discussed in detail elsewhere (Nusca and Michaels, 2003), an empirical one-step reaction (mechanism) was proposed and employed for the earliest version of the model. By adjusting the rate constant of the reaction, it was possible to get the CFD model to produce simulations whose calculations of chamber pressures at steady-state operating conditions matched those observed in test stand firings. However, pressure transients associated with the ignition phase of the ballistic cycle were not well reproduced, and there were questions about how well other results (such as predictions for species concentrations) corresponded to those occurring in the actual motor. Thus, a better representation of the bipropellant's chemical kinetics was considered needed, and the development of a detailed, multistep, finite-rate MMH-RFNA (vs. MMH-IRFNA) mechanism was undertaken.*

An overview of the development of the MMH-RFNA mechanism has been provided previously (McQuaid et al., 2005). Briefly, its construction began in 2003 from sources that included (1) a mechanism that had been assembled to model the combustion of double-base (nitrate ester) and

*Note: RFNA is a mixture of HNO_3, NO_2, and H_2O. To inhibit RFNA's ability to corrode storage containers, a very small amount of HF is added. The resulting mixture is called IRFNA. Because HF is present in such small amounts, its influence in MMH-IRFNA ignition and combustion processes is suspected to be negligible. Therefore, reactions with fluorine-containing species were not included in the mechanism. Without such reactions, the set is more properly called an MMH-RFNA mechanism.

nitramine propellants (Vanderhoff et al., 1992; Anderson et al., 1995), (2) a mechanism that was developed to model the combustion of natural gas (Smith et al., 2003), (3) rate expressions for reactions involving HNO_3, NO_3, N_2O_4 (NTO), and hydrocarbon-NO_x moieties that were identified via a literature search performed specifically for the MMH-RFNA mechanism development effort, and (4) mechanisms Catoire and coworkers developed to model the ignition and combustion of MMH-O_2 and MMH-NTO systems (Catoire et al., 1998; Catoire et al., 2004).

Thermochemical parameters recommended by Catoire and Swihart (2002) for compounds expected to play a role in MMH ignition and combustion were also included. Additional development led to the modification of thermochemical parameters for some species, the inclusion of a $CH_3NHNH_2 + HNO_3$ complexation reaction (McQuaid et al., 2005), and the inclusion of a set of reactions Glarborg and coworkers (1999) developed and employed to model the decomposition of nitromethane.

When the effort to develop the MMH-RFNA mechanism was discontinued in 2005, the mechanism was composed of rate expressions and thermochemical parameters for 513 elementary reactions and 81 species. From a scientific standpoint, additional investigations of other aspects of the mechanism were (and still are) considered warranted (McQuaid et al., 2005), but the expenditure of additional ARL (in-house) resources for such an effort could not be justified. For one, when the CFD model of the ISVE employed a (reduced) chemical kinetics submodel derived from the (full) mechanism, its predictions for the combustion chamber pressure and thrust profiles of ISVE firings agreed with experimental data over the entire ballistic cycle (Nusca and Michaels, 2004; Nusca et al., 2008). In addition, AMRDEC had come to the conclusion that the risks posed by MMH to human health and the environment would make MMH-IRFNA untenable for Army applications for which an ISVE might be utilized. Therefore, AMRDEC started to predicate its ISVE development program on the use of MMH alternatives. With that shift, ARL's basis for developing the mechanism lapsed, and no other Army application for which MMH-RFNA might be used has become apparent since then. With its development discontinued, the 513 reaction-81 species mechanism has come to be viewed as a benchmark.

For several reasons, ARL has not previously published any MMH-RFNA chemical kinetics mechanism in its entirety. When MMH-IRFNA was the primary candidate for fueling ISVEs and the mechanism was an integral aspect of the ISVE development effort, it was recommended that the mechanism's distribution be extremely limited. The shift to MMH-alternatives for the ISVE application reduced the need to restrict the mechanism's distribution, but then there was no particular motivation for undertaking the effort required to produce a reference-quality document for that purpose. Because the primary validation of the mechanism (as a whole) was that a CFD model with a chemical kinetics submodel derived from it produced simulations whose calculations for combustion chamber pressure and thrust agreed with data from MMH-IRFNA fueled rocket motor firings, it would not meet the standards required for publication in a refereed journal. Justification for undertaking the effort to provide it in an ARL technical report was also

lacking. That changed, however, when the U.S. Department of Defense decided to fund two multi university research initiatives (MURIs) on gelled hypergolic propellant spray combustion. Seeking to jump-start their efforts, the MURI groups requested the mechanism. Concluding that the potential benefits of its distribution outweighed the potential negative consequences that can attend the release of a mechanism that has not been rigorously validated and published, ARL distributed it to the groups in October 2008. Consequently, it was considered that a report that provides and discusses the mechanism would be useful for assessing and discussing any proposed refinements. This report is intended to serve that purpose.

In addition, it is anticipated that the MURI groups will employ various methods for reducing their chemical kinetics mechanisms to produce submodels for CFD codes. As such, a common (benchmark) mechanism to which the reduction methods can be applied would be helpful in evaluating their relative merit. (The mechanism had previously been provided to an Aerodyne-Princeton Small Business Technology Transfer [STTR] team for that purpose.) Given its distribution, the mechanism provided here can serve that role as well.

2. Discussion

The MMH-RFNA mechanism that was provided to the MURI groups and the Aerodyne-Princeton STTR team is given in the appendix. As mentioned in the Introduction, the mechanism contains 513 elementary reactions, and except for one case, the rate expressions for the reactions were obtained from open-literature sources. Thermochemical parameters for the species in the mechanism were, likewise, largely obtained from the open literature. In some cases, however, they were developed in-house (McQuaid et al., 2005). In most cases, sets of reactions were taken from mechanisms that had been developed and validated for other systems. This section identifies and discusses the primary sources of the data and the basis of their validation for the application for which they were developed. The numbering of the reactions in this section references table A-2 in the appendix.

2.1 Reactions 1–205

Reactions 1–205 come from a "dark-zone" (DZ) chemical kinetics mechanism that Anderson and coworkers assembled for modeling the combustion of double-base (nitrate ester) and nitramine (gun) propellants (Anderson et al., 1995; Vanderhoff et al., 1992). Because the DZs of flames produced by double-base propellant strands (burning in cigarette fashion at pressures from 1 to 30 atm) contain large quantities of H_2, H_2O, NO, N_2, CO, and CO_2, Anderson et al. (1995) paid considerable attention to identifying a reaction set that could model systems in which these small molecules play prominent roles. Similarly, results from strand burner experiments with

nitramine-containing propellants prompted the inclusion of reactions to account for the production and decomposition of HCN and N_2O. Agreement between predictions based on the DZ mechanism and results from strand burner experiments was good, establishing the mechanism's validity for that application.

Since H_2, H_2O, NO, N_2, CO, CO_2, HCN, and N_2O are all, to varying degrees, expected in MMH-IRFNA combustion, it was natural to include reactions from the DZ mechanism in the MMH-RFNA mechanism. The extracted subset comprises a core of small molecule reactions and species thermochemical parameters that ARL routinely employs in its development of mechanisms for the study of propellant combustion and NO_x emission. Initially developed from a critical review of the literature, this core has since been frequently updated. The bulk of the thermochemical parameters for the species in these reactions was obtained from a database developed at Sandia National Laboratories (Kee et al., 1987). An extensive ARL report that critically reviews the literature on DZ chemistry and provides comparisons between experimentally-based observations and mechanism-based modeling results is being written by Anderson and coworkers (Anderson et al., report in preparation). Full documentation of sources for the most recent version of the DZ mechanism will be provided therein. The data for reactions common to the MMH-RFNA mechanism and the most recent version of the DZ mechanism are mostly the same.

2.2 Reactions 206–351 and 413–427

Reactions 206–351 and 413–427 were taken from GRI-Mech 3.0 (Smith et al., 2009). GRI-Mech 3.0 contains 325 elementary reactions and involves 53 species. It was developed to model the combustion of natural gas and has been extensively validated (as a whole) for that application. Because natural gas is composed primarily of methane, reactions involving small hydrocarbon species are pertinent to its combustion, and the reaction set in GRI-Mech 3.0 reflects this. Because MMH has a methyl (CH_3) group, MMH-RFNA combustion was considered likely to involve similar reactions. Most of the 177 reactions that were extracted from GRI-Mech 3.0 involve $C_xH_yO_z$ species reacting with atoms or diatoms. Some reactions with nitrogen-containing molecules are also present in this (sub)set. Most molecules in reactions 206–351 and 413–427 contain only one or two heavy atoms (i.e., C, N, or O), and none contain more than three. Thermochemical parameters for the molecules involved in these reactions are primarily from Kee et al. (1987).

2.3 Reactions 352–412

Reactions 352–412 were assembled from a literature search focused on identifying rate expressions for elementary reactions that would be relevant for modeling the chemistry of hydrocarbons oxidized by HNO_3 and NO_2. Some of the expressions were extracted from a chemical kinetics mechanism developed to model the combustion of ammonium dinitramide (Anderson, 2001). The thermochemical parameters for the molecules in these reactions are primarily from Kee et al. (1987).

2.4 Reactions 428–443

Reactions 428–443 are small molecule reactions pertinent to hydrocarbon-NO_x, hydrocarbon-N_xH_y, and HCN decomposition chemistry. Their rate expressions were identified through a literature search that was performed subsequent to assembling the characterizations of the reactions discussed in sections 2.1, 2.2, and 2.3. The thermochemical parameters for the molecules in these reactions are primarily from Kee et al. (1987).

2.5 Reactions 444–496

The rate expressions for reactions 444–496 were extracted from mechanisms Catoire and coworkers developed to model MMH-O_2 and MMH-NTO systems (Catoire et al., 1998, 2004). When employed with CHEMKIN to simulate the response of MMH-O_2-Ar mixtures subject to (reflected) shock waves at various pressures and temperatures, the MMH-O_2 mechanism yielded ignition delay times observed experimentally. Similarly, when employed with CHEMKIN to simulate MMH-NTO chemical ignition delays for mixtures at various stoichiometries, temperatures, and pressures, the MMH-NTO mechanism was found to yield results comparable to those predicted by the theory of thermal explosions. Thermochemical parameters for molecules unique to these two mechanisms were obtained from Catoire and Swihart (2002). However, the thermochemical parameters published for $CH_3N(NH_2)NO_2$ and $CH_3N(NH_2)ONO$ were found to be unreasonable and modified (McQuaid et al., 2005). Results from quantum chemistry calculations suggest that the activation energy that Catoire et al. (2004) specified for H-atom abstraction from MMH by NO_2 is slightly low (McQuaid and Ishikawa, 2006), but it was not changed.

2.6 Reaction 497

In developing the MMH-RFNA mechanism, early versions did not produce any significant temperature rise when employed (with CHEMKIN) to simulate the evolution of homogenous MMH-RFNA mixtures initially at temperatures below 600 K. Since such mixtures are known to ignite at temperatures less than 300 K, an explanation was sought. The only possibility that was really considered was the early versions' lack of a direct reaction between MMH and HNO_3. Without such a reaction, HNO_3 acts as a heat sink at temperatures below which it rapidly dissociates to OH and NO_2, soaking up energy from other exothermic processes that have the potential to bootstrap the mixture to a temperature at which ignition will occur.

To address this issue, reaction 497, a complexation reaction between MMH and HNO_3, was added. Given the chemical nature/structure of MMH and HNO_3 (i.e., a base and an acid, respectively), it was clear that a hydrogen bond could form between the two and that the reaction would be strongly exothermic. This was quantified by quantum chemistry calculations. Thermochemical parameters for the MMH-HNO_3 complex (named NAMMH in the mechanism) were derived from a B3LYP/6-31+G(d,p) model. Though this model is not generally

considered sufficient for such purposes, it was considered adequate for obtaining estimates for checking the hypothesized importance of the reaction as an ignition enabler. In the same vein, rate constants for the reaction were specified based simply on the assumption that there was no barrier to the formation of the complex and that it proceeded at a high-pressure limit rate.

With reaction 497 incorporated into the mechanism, ignition-like behavior is observed in simulations of homogenous MMH-RFNA mixtures initially at temperatures as low as 300 K, corroborating the hypothesized importance of a MMH-HNO_3 complexation reaction for the initiation MMH-RFNA mixtures at low temperatures. However, given the level of theory employed to estimate the thermochemical parameters and rate coefficients that characterize it, it is likely that they can be improved. There is also a possibility that rather than simply dissociating back to the reactants, bimolecular reactions of the complex can occur, e.g., with H, OH, or NO_2. Clearly, the mechanism could benefit from further refinement in these areas.

2.7 Reactions 498–513

Reactions 498–513 were taken from a mechanism developed to model shock-induced decomposition of dilute CH_3NO_2-Ar mixtures (Glarborg et al., 1999). Because CH_3 is a likely product of MMH's decomposition and NO_2 is present in RFNA, CH_3NO_2 could possibly form at low temperatures from $CH_3 + NO_2$ recombination, thus making the set's reactions pertinent to MMH-RFNA ignition and combustion. The thermochemical parameters for the molecules in this set are primarily from Kee et al. (1987).

3. Summary

Between 2003 and 2005, a detailed, multistep, finite-rate chemical kinetics mechanism for modeling the ignition and combustion of systems fueled with MMH-RFNA was developed. The mechanism was assembled from reaction rate expressions and thermochemical data that, individually or in sets, were validated for other combustion systems. A lack of relevant experimental data limited the extent to which the mechanism could be validated as a whole, and its development was discontinued prior to resolving some issues that had been raised. Nevertheless, when a subset of the mechanism was employed as a submodel for a CFD model of AMRDEC's ISVE, the CFD model produced simulations whose results for chamber pressure and thrust agreed with ISVE test firing data. As such, the mechanism is considered to have a reasonable measure of validity and should therefore be useful as a starting point for obtaining more refined MMH-RFNA (or MMH-IRFNA) mechanisms.

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Appendix. Mechanism Data Tables

The monomethylhydrazine-red fuming nitric acid (MMH-RFNA) mechanism discussed in this report comprises thermochemical parameters and rate expressions for 81 species and 513 elementary reactions. Thermochemical parameters are given in table A-1, and the rate expressions are given in table A-2. The thermochemical parameters include (1) heat of formation at 298 K [$H_f(298)$], (2) entropy at 298 K [S(298 K)], and (3) the constant pressure heat capacity [$C_P(T)$] as a function of temperature [T].

For reactions whose rates (k) are not a function of pressure, the Arrhenius expression $k = AT^b\exp(-E/RT)$ calculates the rate at a specified temperature from the given frequency factor (A), temperature exponent (b), activation energy (E), and the ideal gas constant (R). For reactions involving a generalized collider species (M) (and whose rates are therefore pressure dependent), an effective collider concentration (C_M) is calculated from the expression $C_M = [p/(RT)]\Sigma_i X_i\eta_i$, where p is the pressure, X_i is the mole fraction, and η_i is the collider efficiency of species i. Collider efficiencies are assumed to be 1.0 unless otherwise specified. Then, one of three expressions is employed for the rate calculation. If "T&H VALUE(S)" is specified, the Tsang and Herron[1] form is used and constants for that form are given, i.e., a_0 and (possibly) a_1. (The standard CHEMKIN interpreter and the subroutine for computing rates have to be modified to perform this computation.) If "TROE centering" is specified, the TROE form is employed, and its parameters are given. If no special form is specified, the Lindemann form is employed. Descriptions of the latter two expression types may be found in the CHEMKIN manual.[2] For reactions that appear in the mechanism more than once, the phrase "declared duplicate reaction" is inserted, and the rate is computed from the sum of the two specified expressions. (The two expressions may or may not actually represent different atomic trajectories.)

[1] Tsang, W.; Herron, J. T. Chemical Kinetic Data Base for Propellant Combustion. I. Reactions Involving NO, NO_2, HNO, HNO_2, HCN and N_2O. *J. Phys. Chem Ref. Data* 20-609–663. (Note that the log expressions used in this source are for base 10 [W. Tsang, private communication] 1991).

[2] Kee, R. J.; Rupley, F. M.; Miller, J. A. *Chemkin II*: *A Fortran Chemical Kinetics Package for the Analysis of Gas-Phase Chemical Kinetics*; SAND89-8009; Sandia National Laboratories: Livermore, CA, 1989.

Table A-1. Thermochemical parameters for species in the MMH-RFNA mechanism (enthalpies in kcal/mol, entropies and heat capacities in cal/K-mole).

SPECIES	HF(298)	S(298)	CP300	CP400	CP500	CP600	CP800	CP1000	CP1500
				CP2000	CP2500	CP3000	CP3500	CP4000	CP5000
O	59.56	38.47	5.23	5.14	5.08	5.05	5.02	5.00	4.98
				4.98	4.98	5.01	5.04	5.09	5.21
O2	.00	49.01	7.01	7.22	7.44	7.65	8.07	8.35	8.72
				9.03	9.29	9.52	9.72	9.90	10.19
N	112.96	36.61	4.97	4.97	4.97	4.97	4.97	4.97	4.97
				4.97	4.98	5.01	5.09	5.21	5.61
NO	21.81	50.37	7.14	7.16	7.29	7.46	7.83	8.12	8.54
				8.78	8.91	8.98	9.03	9.08	9.24
NO2	7.91	57.34	8.83	9.64	10.33	10.93	11.89	12.49	13.17
				13.51	13.65	13.71	13.75	13.80	13.81
NO3	17.00	60.37	11.31	13.32	14.90	16.10	17.59	18.27	19.10
				19.48	19.62	19.66	19.70	19.77	19.76
N2	.00	45.77	6.95	7.01	7.08	7.19	7.50	7.83	8.32
				8.60	8.76	8.85	8.91	8.97	9.05
N2O	19.61	52.55	9.27	10.18	10.94	11.56	12.51	13.12	13.94
				14.36	14.54	14.63	14.69	14.75	14.78
N2O4	2.17	72.74	18.56	21.11	23.18	24.85	27.20	28.51	30.11
				30.89	31.21	31.34	31.43	31.55	31.56
H	52.10	27.39	4.97	4.97	4.97	4.97	4.97	4.97	4.97
				4.97	4.97	4.97	4.97	4.97	4.97
OH	8.89	43.88	7.15	7.10	7.07	7.06	7.13	7.33	7.87
				8.28	8.57	8.78	8.94	9.05	9.26
HO2	3.30	54.76	8.35	8.89	9.46	9.99	10.77	11.38	12.48
				13.33	13.95	14.38	14.66	14.80	14.83
NH	85.50	43.31	6.98	6.98	7.00	7.05	7.22	7.47	8.07
				8.51	8.87	9.18	9.47	9.76	10.27
HNO	25.60	52.80	8.10	8.48	8.98	9.54	10.56	11.40	13.28
				14.69	15.65	16.19	16.38	16.29	15.72
HONO	-18.34	59.59	10.88	12.27	13.39	14.31	15.67	16.56	17.89
				18.64	19.03	19.25	19.39	19.51	19.60
HNO2	-14.15	56.75	9.07	10.43	11.64	12.71	14.46	15.75	17.57
				18.48	18.98	19.23	19.36	19.45	19.64
HNO3	-32.10	63.67	12.83	15.07	16.89	18.34	20.39	21.62	23.38
				24.34	24.82	25.07	25.24	25.40	25.49
NNH	58.57	53.63	8.32	8.83	9.36	9.88	10.85	11.52	12.44
				13.04	13.36	13.48	13.55	13.74	.00
HNNO	55.39	60.56	10.73	12.13	13.29	14.25	15.72	16.72	18.14
				18.83	19.21	19.40	19.49	19.56	19.70
H2	.00	31.21	6.90	6.96	7.00	7.02	7.07	7.21	7.73
				8.18	8.56	8.87	9.13	9.35	9.77
H2O	-57.80	45.10	8.00	8.23	8.44	8.67	9.22	9.87	11.26
				12.22	12.88	13.33	13.64	13.87	14.20
H2O2	-32.53	55.66	10.41	11.44	12.34	13.11	14.29	15.21	16.85
				17.88	18.49	18.86	19.09	19.26	19.47
NH2	45.20	46.60	8.09	8.31	8.60	8.93	9.64	10.36	11.81
				12.84	13.57	14.11	14.51	14.83	15.31
HNOH	21.60	57.81	10.29	11.26	12.14	12.92	14.25	15.28	16.84
				17.63	18.07	18.30	18.42	18.50	18.67
NH2O	15.90	55.71	9.30	10.39	11.36	12.22	13.68	14.84	16.78
				17.88	18.54	18.91	19.12	19.26	19.50
N2H2	45.70	52.18	8.41	9.26	10.32	11.43	13.44	15.08	18.24
				20.08	21.04	21.43	21.53	21.51	21.49
NH3	-10.97	46.04	8.48	9.33	10.08	10.80	12.21	13.53	15.90
				17.40	18.32	18.86	19.16	19.33	19.31
N2H3	52.80	54.63	10.50	12.29	13.84	15.18	17.35	18.98	21.51
				22.81	23.53	23.90	24.09	24.23	24.49

N2H4	22.79	57.03	12.20	14.76	16.83	18.52	21.12	23.04	26.33
				28.28	29.38	30.02	30.43	30.75	31.06
C	171.31	37.76	4.98	4.98	4.97	4.97	4.97	4.97	4.97
				5.01	5.08	5.17	5.26	5.34	5.46
CO	-26.42	47.21	6.95	7.03	7.14	7.27	7.61	7.95	8.41
				8.67	8.81	8.89	8.96	9.01	9.09
CO2	-94.06	51.08	8.91	9.86	10.65	11.31	12.32	12.99	13.93
				14.44	14.71	14.86	14.99	15.12	15.28
CN	104.01	48.41	6.97	7.03	7.15	7.32	7.71	8.02	8.49
				9.01	9.54	10.03	10.45	10.76	10.99
NCO	31.30	55.51	9.59	10.49	11.23	11.84	12.75	13.35	14.08
				14.46	14.64	14.71	14.73	14.76	14.89
NCN	107.60	54.77	10.58	11.50	12.22	12.78	13.52	13.96	14.45
				14.64	14.74	14.79	14.81	14.85	.00
NCNO	78.09	63.84	12.93	13.89	14.77	15.56	16.82	17.56	18.53
				19.14	19.43	19.51	19.55	19.77	.00
CH	142.01	43.72	6.95	7.00	7.05	7.11	7.37	7.78	8.75
				9.36	9.72	9.90	9.98	10.02	10.14
HCO	10.04	53.62	8.27	8.72	9.24	9.78	10.74	11.49	12.54
				13.16	13.49	13.67	13.78	13.89	14.13
HOCO	-46.29	60.12	10.78	12.19	13.34	14.29	15.67	16.57	17.70
				18.16	18.43	18.56	18.62	18.72	.00
HCN	31.89	48.24	8.59	9.36	9.97	10.48	11.31	12.01	13.20
				13.94	14.38	14.64	14.79	14.91	15.11
HNC	45.20	49.20	8.60	9.32	9.94	10.47	11.34	12.02	13.18
				13.82	14.19	14.39	14.50	14.57	14.71
HOCN	-3.53	59.26	10.56	11.45	12.27	13.02	14.26	15.19	16.55
				17.39	17.89	18.14	18.29	18.51	.00
HNCO	-28.22	56.94	10.79	12.11	13.14	13.97	15.20	16.14	17.59
				18.45	18.93	19.18	19.32	19.42	19.62
HCNO	38.43	53.80	11.63	13.05	14.25	15.22	16.56	17.33	18.68
				19.56	20.03	20.21	20.31	20.61	.00
CH2	92.49	46.72	8.25	8.55	8.88	9.23	9.93	10.57	11.74
				12.54	13.00	13.22	13.35	13.58	.00
CH2(S)	101.51	45.10	8.07	8.30	8.60	8.98	9.85	10.61	11.83
				12.64	13.09	13.28	13.39	13.64	.00
CH2O	-25.95	52.28	8.47	9.36	10.44	11.52	13.37	14.82	17.01
				18.10	18.66	19.02	19.22	.00	.00
H2CN	59.11	53.60	9.16	10.32	11.42	12.47	14.24	15.42	17.13
				18.25	18.84	19.07	19.19	19.55	.00
H2CNO2	36.47	65.59	15.21	17.96	20.14	21.87	24.33	25.91	28.11
				29.10	29.69	30.00	30.17	30.38	.00
CH3	34.82	46.38	9.23	10.09	10.83	11.52	12.87	14.12	16.27
				17.55	18.29	18.71	18.98	19.19	19.40
CH3O	3.90	54.61	9.08	10.79	12.43	13.98	16.63	18.60	21.51
				23.26	24.21	24.67	.00	.00	.00
CH2OH	-4.10	58.88	11.32	12.94	14.38	15.62	17.54	18.79	20.95
				22.40	23.23	23.60	23.82	24.27	.00
CH2NH	21.85	55.95	9.47	10.94	12.42	13.86	16.48	18.62	21.72
				23.30	24.18	24.64	24.89	25.06	25.39
CH3NO	18.95	63.48	12.05	14.19	16.11	17.84	20.73	22.98	26.33
				27.97	28.96	29.47	29.74	30.11	.00
CH3NO2	-16.84	72.04	13.47	16.60	19.28	21.58	25.21	27.88	31.75
				33.59	34.71	35.28	35.58	35.99	.00
CH3ONO	-15.25	66.88	15.43	18.38	20.86	22.96	26.25	28.66	32.29
				34.08	35.18	35.74	36.00	36.30	.00
CH3ONO2	-26.05	71.64	17.72	21.48	24.62	27.24	31.23	34.02	37.81
				39.39	40.31	40.73	40.92	41.26	.00
CH3NN	56.09	63.62	13.00	14.97	16.87	18.63	21.63	23.72	26.92
				28.81	29.85	30.38	30.65	30.85	31.28
CH4	-17.90	44.47	8.43	9.84	11.14	12.41	15.00	17.25	20.63
				22.58	23.65	24.23	24.60	24.90	25.17

CH3OH	-48.06	57.28	10.51	12.40	14.25	16.01	19.07	21.40	25.02
				27.25	28.51	29.16	29.47	29.67	30.27
CH3NH	44.83	56.40	11.36	13.39	15.48	17.40	20.42	22.80	26.40
				28.53	29.67	30.23	30.53	30.75	31.24
CH3NNH	42.49	61.80	12.96	15.52	18.07	20.47	24.48	27.20	31.38
				33.86	35.21	35.90	36.26	36.52	37.08
CH3NNH2	49.49	65.35	15.28	18.36	21.24	23.88	28.24	31.28	36.07
				38.95	40.57	41.42	41.88	42.21	42.87
CH3N(NH2)N	24.18	78.95	23.99	28.88	33.21	36.98	42.96	46.88	52.69
				56.13	58.02	58.98	59.49	59.86	60.64
CH3N(NH2)O	38.49	80.06	25.54	30.45	34.60	38.13	43.70	47.46	53.00
				56.30	58.12	59.06	59.56	59.92	60.67
CH3NHNH2	22.62	63.93	15.47	19.29	22.67	25.69	30.83	34.60	40.32
				43.80	45.79	46.85	47.44	47.85	48.62
NAMMH	-23.25	95.88	30.43	36.35	41.82	46.74	54.70	59.92	67.62
				72.21	74.73	76.03	76.71	77.19	78.21
C2N2	73.88	57.73	13.63	14.71	15.59	16.32	17.45	18.24	19.41
				20.02	20.31	20.44	20.54	20.63	20.67
C2H	135.01	49.56	8.90	9.63	10.22	10.72	11.54	12.18	13.31
				14.12	14.77	15.31	15.75	15.99	.00
HCCO	42.45	60.74	12.65	13.47	14.23	14.92	16.07	16.83	17.98
				18.74	19.14	19.30	19.39	19.64	.00
C2H2	54.20	48.02	10.62	11.99	13.08	13.95	15.27	16.31	18.27
				19.52	20.30	20.82	21.21	21.55	22.05
CH2CO	-12.40	57.79	12.43	14.17	15.67	16.91	18.79	20.24	22.44
				23.78	24.52	24.89	25.07	25.18	25.54
HCCOH	20.43	58.71	13.22	14.78	16.16	17.35	19.15	20.30	22.29
				23.62	24.37	24.71	24.90	25.32	.00
C2H3	68.42	55.33	9.57	11.19	12.78	14.31	16.98	18.75	21.26
				23.07	24.19	24.74	24.89	24.88	25.74
CH2CHO	6.00	64.01	13.18	15.15	16.96	18.60	21.30	23.34	26.35
				28.16	29.14	29.61	29.82	29.96	30.43
C2H4	12.54	52.38	10.23	12.79	14.94	16.83	20.05	22.51	26.22
				28.33	29.46	30.07	30.46	30.79	31.07
CH3CHO	-39.72	63.09	13.26	15.78	18.29	20.58	24.16	26.91	30.96
				33.30	34.53	35.12	35.42	35.65	36.19
C2H4O	-12.58	58.09	11.38	14.91	17.93	20.51	24.58	27.50	31.78
				34.03	35.31	36.00	36.37	36.62	37.10
C2H5	28.02	60.14	11.32	13.60	15.95	18.29	22.58	25.50	29.56
				32.45	34.24	35.09	35.30	35.27	36.66
C2H6	-20.04	54.73	12.58	15.69	18.62	21.30	25.82	29.30	34.61
				37.92	39.83	40.88	41.48	41.93	.00
CH3NNCH3	36.41	68.72	18.81	23.14	27.07	30.59	36.35	40.51	46.91
				50.22	51.93	52.95	53.69	54.03	.00

Table A-2. Rate Parameters for Elementary Reactions in the MMH-RFNA Mechanism.

REACTIONS CONSIDERED	(k = A T**b exp(-E/RT)) A	b	E
1. NO2(+M)=NO+O(+M)	7.600E+18	-1.27	73290.0
Low pressure limit: 0.24700E+29 -0.33700E+01 0.74800E+05			
T&H VALUES 0.95000E+00 -0.10000E-03			
N2O Enhanced by 1.500E+00			
H2O Enhanced by 4.400E+00			
N2 Enhanced by 1.000E+00			
CO2 Enhanced by 2.300E+00			
2. N2O(+M)=N2+O(+M)	1.260E+12	0.00	62620.0
Low pressure limit: 0.59700E+15 0.00000E+00 0.56640E+05			
N2O Enhanced by 5.000E+00			
H2O Enhanced by 9.000E+00			
N2 Enhanced by 1.000E+00			
CO2 Enhanced by 3.200E+00			
O2 Enhanced by 8.200E-01			
3. H+NO(+M)=HNO(+M)	1.520E+15	-0.41	0.0
Low pressure limit: 0.40000E+21 -0.17500E+01 0.00000E+00			
N2O Enhanced by 5.000E+00			
H2O Enhanced by 5.000E+00			
N2 Enhanced by 1.000E+00			
CO2 Enhanced by 1.300E+00			
4. NO+OH(+M)=HONO(+M)	1.988E+12	-0.05	-721.0
Low pressure limit: 0.50800E+24 -0.25100E+01 -0.67600E+02			
T&H VALUE 0.62000E+00			
N2O Enhanced by 5.000E+00			
H2O Enhanced by 8.300E+00			
N2 Enhanced by 1.000E+00			
CO2 Enhanced by 1.500E+00			
5. HCN(+M)=H+CN(+M)	8.300E+17	-0.93	123800.0
Low pressure limit: 0.35700E+27 -0.26000E+01 0.12490E+06			
T&H VALUES 0.95000E+00 -0.10000E-03			
N2O Enhanced by 5.000E+00			
H2O Enhanced by 5.000E+00			
N2 Enhanced by 1.000E+00			
CO2 Enhanced by 1.600E+00			
6. CN+CN(+M)=C2N2(+M)	5.660E+12	0.00	0.0
Low pressure limit: 0.34300E+26 -0.26100E+01 0.00000E+00			
T&H VALUE 0.50000E+00			
N2O Enhanced by 5.000E+00			
H2O Enhanced by 5.000E+00			
N2 Enhanced by 1.000E+00			
CO2 Enhanced by 1.600E+00			
7. HNCO(+M)=NH+CO(+M)	6.000E+13	0.00	99800.0
Low pressure limit: 0.21700E+29 -0.31000E+01 0.10190E+06			
T&H VALUES 0.90000E+00 -0.20000E-03			
N2O Enhanced by 5.000E+00			
H2O Enhanced by 5.000E+00			
N2 Enhanced by 1.000E+00			
CO2 Enhanced by 1.600E+00			
8. HCN+H(+M)=H2CN(+M)	3.310E+13	0.00	4844.0
Low pressure limit: 0.16000E+25 -0.27300E+01 0.76600E+04			
T&H VALUES 0.95000E+00 -0.10000E-03			

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      N2O              Enhanced by    5.000E+00
      H2O              Enhanced by    5.000E+00
      N2               Enhanced by    1.000E+00
      CO2              Enhanced by    2.000E+00
 9. CN+NO(+M)=NCNO(+M)                          3.980E+13    0.00     0.0
    Low pressure limit:  0.15600E+37 -0.62000E+01  0.48780E+04
    T&H VALUE  0.65000E+00
      N2O              Enhanced by    5.000E+00
      H2O              Enhanced by    5.000E+00
      N2               Enhanced by    1.000E+00
      CO2              Enhanced by    2.000E+00
10. CN+M=C+N+M                                  2.500E+14    0.00  141100.0
      N2               Enhanced by    1.500E+00
      CO2              Enhanced by    2.400E+00
11. NO+M=N+O+M                                  1.400E+15    0.00  148430.0
      N2               Enhanced by    1.000E+00
      H2               Enhanced by    2.200E+00
      H2O              Enhanced by    6.700E+00
      CO2              Enhanced by    3.000E+00
      N2O              Enhanced by    2.200E+00
12. N2+M=N+N+M                                  3.710E+21   -1.60  225000.0
13. NO2+N=N2O+O                                 3.490E+12    0.00    -437.0
14. NO2+NO2=NO+NO3                              9.640E+09    0.73   20920.0
15. NO2+NO2=NO+NO+O2                            4.510E+12    0.00   27600.0
16. NO2+NO3=NO+NO2+O2                           2.710E+10    0.00    2500.0
17. HNO+NO=N2O+OH                               1.700E+13    0.00   29590.0
18. HNO+O2=HO2+NO                               1.000E+13    0.00   25000.0
19. HNO+NO2=HONO+NO                             4.420E+04    2.64    4042.0
20. HONO+O=OH+NO2                               1.200E+13    0.00    5961.0
21. HONO+OH=H2O+NO2                             1.270E+10    1.00     135.0
22. HONO+NH2=NO2+NH3                            1.000E+10    1.00       0.0
23. HNO+O=OH+NO                                 3.610E+13    0.00       0.0
24. NH+O=NO+H                                   5.500E+13    0.00       0.0
25. NH+O=N+OH                                   3.720E+13    0.00       0.0
26. NH+NH=N2+H+H                                5.100E+13    0.00       0.0
27. NH+M=N+H+M                                  2.650E+14    0.00   75510.0
28. CH+O2=HCO+O                                 3.300E+13    0.00       0.0
29. CH+O=CO+H                                   5.700E+13    0.00       0.0
30. CH+OH=HCO+H                                 3.000E+13    0.00       0.0
31. CH+CO2=HCO+CO                               3.400E+12    0.00     690.0
32. CH+H=C+H2                                   1.500E+14    0.00       0.0
33. C+O2=CO+O                                   2.000E+13    0.00       0.0
34. C+OH=CO+H                                   5.000E+13    0.00       0.0
35. HCO+OH=H2O+CO                               1.000E+14    0.00       0.0
36. HCO+M=H+CO+M                                2.500E+14    0.00   16802.0
      CO               Enhanced by    1.900E+00
      H2               Enhanced by    1.900E+00
      CO2              Enhanced by    3.000E+00
      H2O              Enhanced by    5.000E+00
37. HCO+H=CO+H2                                 1.190E+13    0.25      0.0
38. HCO+O=CO+OH                                 3.000E+13    0.00      0.0
39. HCO+O=CO2+H                                 3.000E+13    0.00      0.0
40. HCO+O2=HO2+CO                               3.300E+13   -0.40      0.0
41. CO+O(+M)=CO2(+M)                            1.800E+10    0.00   2380.0
    Low pressure limit:  0.13500E+25 -0.27900E+01  0.41900E+04
    T&H VALUE  0.10000E+01
      H2O              Enhanced by    1.200E+01
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       H2              Enhanced by    2.500E+00
       CO              Enhanced by    1.900E+00
       CO2             Enhanced by    3.800E+00
       N2O             Enhanced by    5.000E+00
42. CO+OH=CO2+H                             1.510E+07    1.30    -758.0
43. CO+O2=CO2+O                             2.530E+12    0.00   47688.0
44. HO2+CO=CO2+OH                           5.800E+13    0.00   22934.0
45. O+HCCO=H+2CO                            1.000E+14    0.00       0.0
46. HCCO+O2=2CO+OH                          1.600E+12    0.00     854.0
47. OH+H2=H2O+H                             2.160E+08    1.50    3430.0
48. O2+H=O+OH                               3.520E+16   -0.70   17070.0
49. O+H2=OH+H                               5.060E+04    2.67    6290.0
50. H+O2+M=HO2+M                            3.610E+17   -0.72       0.0
       H2O             Enhanced by    1.860E+01
       CO2             Enhanced by    4.200E+00
       H2              Enhanced by    2.900E+00
       CO              Enhanced by    2.100E+00
       N2              Enhanced by    1.300E+00
51. OH+HO2=H2O+O2                           7.500E+12    0.00       0.0
52. H+HO2=2OH                               1.690E+14    0.00     874.0
53. H+HO2=H2+O2                             4.280E+13    0.00    1411.0
54. H+HO2=O+H2O                             3.010E+13    0.00    1721.0
55. O+HO2=O2+OH                             1.400E+13    0.00    1073.0
56. OH+OH=H2O+O                             3.570E+04    2.40    2112.0
57. 2H+M=H2+M                               1.000E+18   -1.00       0.0
       H2              Enhanced by    0.000E+00
       H2O             Enhanced by    0.000E+00
       CO2             Enhanced by    0.000E+00
58. 2H+H2=2H2                               9.200E+16   -0.60       0.0
59. 2H+H2O=H2+H2O                           6.000E+19   -1.25       0.0
60. 2H+CO2=H2+CO2                           5.490E+20   -2.00       0.0
61. H+OH+M=H2O+M                            1.600E+22   -2.00       0.0
       H2O             Enhanced by    5.000E+00
62. H+O+M=OH+M                              6.200E+16   -0.60       0.0
       H2O             Enhanced by    5.000E+00
63. O+O+M=O2+M                              1.890E+13    0.00   -1788.0
64. 2HO2=H2O2+O2                            1.800E+12    0.00       0.0
65. H2O2+H=HO2+H2                           4.820E+13    0.00    7948.0
66. H2O2+H=OH+H2O                           2.410E+13    0.00    3975.0
67. H2O2+O=HO2+OH                           9.630E+06    2.00    3974.0
68. H2O2+OH=H2O+HO2                         1.750E+12    0.00     318.0
69. CH+N2=NCN+H                             2.220E+07    1.48   23367.0
70. H+NCN=HCN+N                             1.890E+14    0.00    8425.0
71. NCN+N=CN+N2                             2.000E+13    0.00       0.0
72. CN+N=C+N2                               1.040E+15   -0.50       0.0
73. C+NO=CN+O                               6.600E+13    0.00       0.0
74. HCCO+NO=HCNO+CO                         2.000E+13    0.00       0.0
75. CH+N=CN+H                               1.300E+13    0.00       0.0
76. HCCO+N=HCN+CO                           5.000E+13    0.00       0.0
77. HCN+OH=CN+H2O                           3.900E+06    1.83   10290.0
78. OH+HCN=HNCO+H                           1.980E-03    4.00    1000.0
79. OH+HCN=NH2+CO                           7.830E-04    4.00    4000.0
80. HCN+O=NCO+H                             1.380E+04    2.64    4980.0
81. HCN+O=NH+CO                             3.450E+03    2.64    4980.0
82. HCN+O=CN+OH                             2.700E+09    1.58   26600.0
83. CN+H2=HCN+H                             3.610E+08    1.55    3000.0
84. CN+O=CO+N                               2.050E+13    0.00     417.0
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85.	CN+O2=NCO+O			2.600E+14	-0.50	0.0
86.	CN+OH=NCO+H			4.000E+13	0.00	0.0
87.	CN+HCN=C2N2+H			1.510E+07	1.71	1530.0
88.	CN+NO2=NCO+NO			6.160E+15	-0.75	344.0
89.	CN+CO2=NCO+CO			3.670E+06	2.16	26900.0
90.	CN+N2O=NCN+NO			2.400E+13	0.00	13330.0
91.	C2N2+O=NCO+CN			4.570E+12	0.00	8880.0
92.	NO+HO2=NO2+OH			2.110E+12	0.00	-479.0
93.	NO2+H=NO+OH			1.300E+14	0.00	361.0
94.	NO2+O=NO+O2			3.900E+12	0.00	-238.0
95.	NCO+H=NH+CO			5.400E+13	0.00	0.0
96.	NCO+O=NO+CO			4.520E+13	0.00	0.0
97.	NCO+O2=NO+CO2			2.000E+12	0.00	20000.0
98.	NCO+N=N2+CO			2.000E+13	0.00	0.0
99.	NCO+OH=NO+CO+H			2.000E+13	0.00	7500.0
100.	NCO+M=N+CO+M			1.140E+23	-1.95	59930.0
	N2O	Enhanced by	5.000E+00			
	H2O	Enhanced by	5.000E+00			
	N2	Enhanced by	1.000E+00			
	CO2	Enhanced by	1.500E+00			
101.	NCO+NO=N2O+CO			3.980E+19	-2.19	1743.0
102.	NCO+NO=CO2+N2			1.460E+21	-2.74	1824.0
103.	NCO+H2=HNCO+H			2.070E+06	2.00	6020.0
104.	NCO+NO2=CO2+N2O			1.950E+13	-0.26	-620.0
105.	NCO+NO2=CO+NO+NO			1.770E+12	-0.26	-620.0
106.	NH+O2=HNO+O			4.610E+05	2.00	6500.0
107.	NH+O2=NO+OH			1.280E+06	1.50	100.0
108.	NH+NO=N2O+H			3.500E+14	-0.46	16.1
109.	NH+NO=N2+OH			2.160E+13	-0.23	0.0
110.	N2O+OH=N2+HO2			1.290E-02	4.72	36561.0
111.	N2O+H=N2+OH			1.300E+11	0.94	15210.0
112.	NNH+O=N2O+H			1.400E+14	-0.40	477.0
113.	NNH+O=NO+NH			3.300E+14	-0.23	-1013.0
114.	N2O+O=N2+O2			3.692E+12	0.00	15940.0
115.	N2O+O=NO+NO			9.155E+13	0.00	27680.0
116.	H+HNO=NH+OH			3.000E+14	0.00	18000.0
117.	NH+OH=N+H2O			5.000E+11	0.50	2000.0
118.	NH+N=N2+H			3.000E+13	0.00	0.0
119.	N+H2=NH+H			2.330E+14	0.00	30830.0
120.	NH2+O=HNO+H			4.600E+13	0.00	0.0
121.	NH2+O=NH+OH			7.000E+12	0.00	0.0
	Declared duplicate reaction...					
122.	NH2+O=NH+OH			3.330E+08	1.50	5077.0
	Declared duplicate reaction...					
123.	NH2+OH=NH+H2O			4.000E+06	2.00	1000.0
124.	NH2+H=NH+H2			4.000E+13	0.00	3650.0
125.	NH2+NH=N2H2+H			1.500E+15	-0.50	0.0
126.	NH2+N=N2+H+H			7.200E+13	0.00	0.0
127.	NH2+O2=HNO+OH			4.500E+12	0.00	25000.0
128.	NH2+NH2=NH+NH3			5.000E+13	0.00	10000.0
129.	NH2+NH2=N2H3+H			1.790E+13	-0.35	11320.0
130.	NH2+NH2+M=N2H4+M			2.980E+47	-9.44	9680.0
131.	NH+NO2=N2O+OH			4.000E+12	0.00	0.0
132.	NH+NO2=NO+HNO			5.700E+12	0.00	0.0
133.	N2H4+H=N2H3+H2			4.900E+12	0.00	2130.0
134.	N2H4+O=N2H3+OH			6.700E+08	1.50	2851.0

135.	N2H4+OH=N2H3+H2O			4.800E+06	2.00	-646.0
136.	N2H3+H=N2H2+H2			2.400E+08	1.50	-10.0
137.	N2H3+O=NH2+HNO			3.000E+13	0.00	0.0
138.	N2H3+O=N2H2+OH			1.700E+08	1.50	-646.0
139.	N2H3+OH=N2H2+H2O			1.200E+06	2.00	-1192.0
140.	N2H3+NH2=N2H2+NH3			9.200E+05	1.94	-1152.0
141.	N2H3+HO2=N2H2+H2O2			2.900E+04	2.69	-1600.0
142.	N2H3+HO2=N2H4+O2			9.200E+05	1.94	2126.0
143.	N2H2+M=NNH+H+M			5.000E+16	0.00	50000.0
	H2O	Enhanced by	1.500E+01			
	O2	Enhanced by	2.000E+00			
	N2	Enhanced by	2.000E+00			
	H2	Enhanced by	2.000E+00			
144.	N2H2+H=NNH+H2			5.000E+13	0.00	1000.0
145.	N2H2+O=NH2+NO			1.000E+13	0.00	0.0
146.	N2H2+O=NNH+OH			2.000E+13	0.00	1000.0
147.	N2H2+OH=NNH+H2O			1.000E+13	0.00	1000.0
148.	N2H2+NH=NNH+NH2			1.000E+13	0.00	1000.0
149.	N2H2+NH2=NH3+NNH			1.000E+13	0.00	1000.0
150.	NH2+NO=NNH+OH			2.290E+10	0.42	-815.0
151.	NH2+NO=N2+H2O			2.770E+20	-2.65	1258.0
152.	NH3+OH=NH2+H2O			2.040E+06	2.04	566.0
153.	NH3+H=NH2+H2			5.420E+05	2.40	9917.0
154.	NH3+O=NH2+OH			9.400E+06	1.94	6460.0
155.	NH3(+M)=NH2+H(+M)			5.500E+15	0.00	107792.0
	Low pressure limit:	0.22000E+17	0.00000E+00	0.93470E+05		
156.	NNH+NO=N2+HNO			2.000E+13	0.00	0.0
157.	NNH+H=N2+H2			1.000E+14	0.00	0.0
158.	NNH+OH=N2+H2O			5.000E+13	0.00	0.0
159.	NNH+NH2=N2+NH3			5.000E+13	0.00	0.0
160.	NNH+NH=N2+NH2			5.000E+13	0.00	0.0
161.	HNO+OH=NO+H2O			1.295E+07	1.88	-958.0
162.	H+HNO=H2+NO			4.460E+11	0.72	655.0
163.	HNO+NH2=NH3+NO			2.000E+13	0.00	1000.0
164.	N+NO=N2+O			3.270E+12	0.30	0.0
165.	O+NO=N+O2			3.800E+09	1.00	41375.0
166.	NO+H=N+OH			1.700E+14	0.00	48800.0
167.	HNO+HNO=N2O+H2O			3.630E-03	3.98	1190.0
168.	HNC+O=NH+CO			5.440E+12	0.00	0.0
169.	HNC+O=H+NCO			1.600E+01	3.08	-224.0
170.	HNC+OH=HNCO+H			2.800E+13	0.00	3696.0
171.	N2O+NO=N2+NO2			4.290E+13	0.00	47130.0
172.	NO+NO+NO=N2O+NO2			1.070E+10	0.00	26800.0
173.	HOCO+M=OH+CO+M			2.190E+23	-1.89	35270.0
174.	HNC+OH=CN+H2O			1.500E+12	0.00	7680.0
175.	HNC+NO2=HNCO+NO			1.000E+12	0.00	32000.0
176.	HNCO+O=CO2+NH			9.800E+07	1.41	8524.0
177.	HNCO+O=NCO+OH			2.200E+06	2.11	11430.0
178.	HNCO+O=HNO+CO			1.490E+08	1.57	44010.0
179.	HNCO+OH=H2O+NCO			4.790E+05	2.00	2560.0
180.	HNCO+OH=NH2+CO2			1.600E+05	2.00	2560.0
181.	HNCO+HO2=NCO+H2O2			3.000E+11	0.00	23700.0
182.	HNCO+NH=NH2+NCO			2.000E+13	0.00	19300.0
183.	HNCO+H=NH2+CO			2.250E+07	1.70	3800.0
184.	HNCO+NO2=HNNO+CO2			2.500E+12	0.00	26000.0
185.	CH+NO=HCN+O			1.100E+14	0.00	0.0
186.	CN+NO=NCO+N			5.500E+12	0.00	30620.0

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187. CN+NO=N2+CO                                  3.900E+11    0.00   27820.0
188. CN+NO=NCN+O                                  1.800E+13    0.00   38190.0
189. CO+NO2=NO+CO2                                9.040E+13    0.00   33780.0
190. CH+NO2=HCO+NO                                1.010E+14    0.00       0.0
191. H2+NO2=HONO+H                                1.300E+04    2.76   29770.0
192. HONO+H=HNO+OH                                5.630E+10    0.86    4969.0
193. HONO+H=H2O+NO                                8.130E+06    1.89    3847.0
194. 2HONO=NO+NO2+H2O                             3.490E-01    3.64   12140.0
195. NNH(+M)=N2+H(+M)                             4.100E+09    1.13    5186.0
     Low pressure limit:  0.10000E+14  0.50000E+00  0.30600E+04
        N2O              Enhanced by    5.000E+00
        H2O              Enhanced by    9.000E+00
        N2               Enhanced by    1.000E+00
        O2               Enhanced by    8.200E-01
        HNO3             Enhanced by    5.000E+00
        NH3              Enhanced by    5.000E+00
        NO3              Enhanced by    5.000E+00
     Declared duplicate reaction...
196. NNH=N2+H                                     3.000E+08    0.00       0.0
     Declared duplicate reaction...
197. HCN+M=HNC+M                                  4.360E+26   -3.34   50194.0
198. HNO+NO+NO=HNNO+NO2                           1.700E+11    0.00    2100.0
199. HNNO+NO=NNH+NO2                              3.200E+12    0.00     270.0
200. HNNO+NO=N2+HONO                              2.600E+11    0.00     810.0
201. HNNO+M=H+N2O+M                               2.200E+15    0.00   21600.0
202. HNNO+M=N2+OH+M                               1.000E+15    0.00   25600.0
203. HNNO+OH=H2O+N2O                              2.000E+13    0.00       0.0
204. HNNO+H=H2+N2O                                2.000E+13    0.00       0.0
205. HCO+NO=HNO+CO                                7.230E+12    0.00       0.0
206. O+CH2<=>H+HCO                                8.000E+13    0.00       0.0
207. O+CH2(S)<=>H2+CO                             1.500E+13    0.00       0.0
208. O+CH2(S)<=>H+HCO                             1.500E+13    0.00       0.0
209. O+CH3<=>H+CH2O                               5.060E+13    0.00       0.0
210. O+CH4<=>OH+CH3                               1.020E+09    1.50    8600.0
211. O+CH2O<=>OH+HCO                              3.900E+13    0.00    3540.0
212. O+CH2OH<=>OH+CH2O                            1.000E+13    0.00       0.0
213. O+CH3O<=>OH+CH2O                             1.000E+13    0.00       0.0
214. O+CH3OH<=>OH+CH2OH                           3.880E+05    2.50    3100.0
215. O+CH3OH<=>OH+CH3O                            1.300E+05    2.50    5000.0
216. O+C2H<=>CH+CO                                5.000E+13    0.00       0.0
217. O+C2H2<=>H+HCCO                              1.350E+07    2.00    1900.0
218. O+C2H2<=>OH+C2H                              4.600E+19   -1.41   28950.0
219. O+C2H2<=>CO+CH2                              6.940E+06    2.00    1900.0
220. O+C2H3<=>H+CH2CO                             3.000E+13    0.00       0.0
221. O+C2H4<=>CH3+HCO                             1.250E+07    1.83     220.0
222. O+C2H5<=>CH3+CH2O                            2.240E+13    0.00       0.0
223. O+C2H6<=>OH+C2H5                             8.980E+07    1.92    5690.0
224. O+CH2CO<=>OH+HCCO                            1.000E+13    0.00    8000.0
225. O+CH2CO<=>CH2+CO2                            1.750E+12    0.00    1350.0
226. O2+CH2O<=>HO2+HCO                            1.000E+14    0.00   40000.0
227. H+CH2(+M)<=>CH3(+M)                          6.000E+14    0.00       0.0
     Low pressure limit:  0.10400E+27 -0.27600E+01  0.16000E+04
     TROE centering:      0.56200E+00  0.91000E+02  0.58360E+04  0.85520E+04
        H2               Enhanced by    2.000E+00
        H2O              Enhanced by    6.000E+00
        CH4              Enhanced by    2.000E+00
        CO               Enhanced by    1.500E+00
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        CO2              Enhanced by    2.000E+00
        C2H6             Enhanced by    3.000E+00
228. H+CH2(S)<=>CH+H2                          3.000E+13    0.00       0.0
229. H+CH3(+M)<=>CH4(+M)                       1.390E+16   -0.53     536.0
     Low pressure limit:  0.26200E+34 -0.47600E+01  0.24400E+04
     TROE centering:      0.78300E+00  0.74000E+02  0.29410E+04  0.69640E+04
        H2               Enhanced by    2.000E+00
        H2O              Enhanced by    6.000E+00
        CH4              Enhanced by    3.000E+00
        CO               Enhanced by    1.500E+00
        CO2              Enhanced by    2.000E+00
        C2H6             Enhanced by    3.000E+00
230. H+CH4<=>CH3+H2                            6.600E+08    1.62   10840.0
231. H+HCO(+M)<=>CH2O(+M)                      1.090E+12    0.48    -260.0
     Low pressure limit:  0.24700E+25 -0.25700E+01  0.42500E+03
     TROE centering:      0.78240E+00  0.27100E+03  0.27550E+04  0.65700E+04
        H2               Enhanced by    2.000E+00
        H2O              Enhanced by    6.000E+00
        CH4              Enhanced by    2.000E+00
        CO               Enhanced by    1.500E+00
        CO2              Enhanced by    2.000E+00
        C2H6             Enhanced by    3.000E+00
232. H+CH2O(+M)<=>CH2OH(+M)                    5.400E+11    0.45    3600.0
     Low pressure limit:  0.12700E+33 -0.48200E+01  0.65300E+04
     TROE centering:      0.71870E+00  0.10300E+03  0.12910E+04  0.41600E+04
        H2               Enhanced by    2.000E+00
        H2O              Enhanced by    6.000E+00
        CH4              Enhanced by    2.000E+00
        CO               Enhanced by    1.500E+00
        CO2              Enhanced by    2.000E+00
        C2H6             Enhanced by    3.000E+00
233. H+CH2O<=>HCO+H2                           5.740E+07    1.90    2742.0
234. H+CH2OH(+M)<=>CH3OH(+M)                   1.055E+12    0.50      86.0
     Low pressure limit:  0.43600E+32 -0.46500E+01  0.50800E+04
     TROE centering:      0.60000E+00  0.10000E+03  0.90000E+05  0.10000E+05
        H2               Enhanced by    2.000E+00
        H2O              Enhanced by    6.000E+00
        CH4              Enhanced by    2.000E+00
        CO               Enhanced by    1.500E+00
        CO2              Enhanced by    2.000E+00
        C2H6             Enhanced by    3.000E+00
235. H+CH2OH<=>H2+CH2O                         2.000E+13    0.00       0.0
236. H+CH2OH<=>OH+CH3                          1.650E+11    0.65    -284.0
237. H+CH2OH<=>CH2(S)+H2O                      3.280E+13   -0.09     610.0
238. H+CH3O(+M)<=>CH3OH(+M)                    2.430E+12    0.52      50.0
     Low pressure limit:  0.46600E+42 -0.74400E+01  0.14080E+05
     TROE centering:      0.70000E+00  0.10000E+03  0.90000E+05  0.10000E+05
        H2               Enhanced by    2.000E+00
        H2O              Enhanced by    6.000E+00
        CH4              Enhanced by    2.000E+00
        CO               Enhanced by    1.500E+00
        CO2              Enhanced by    2.000E+00
        C2H6             Enhanced by    3.000E+00
239. H+CH3O<=>H+CH2OH                          4.150E+07    1.63    1924.0
240. H+CH3O<=>H2+CH2O                          2.000E+13    0.00       0.0
241. H+CH3O<=>OH+CH3                           1.500E+12    0.50    -110.0
242. H+CH3O<=>CH2(S)+H2O                       2.620E+14   -0.23    1070.0
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243. H+CH3OH<=>CH2OH+H2                          1.700E+07    2.10    4870.0
244. H+CH3OH<=>CH3O+H2                           4.200E+06    2.10    4870.0
245. H+C2H(+M)<=>C2H2(+M)                        1.000E+17   -1.00       0.0
     Low pressure limit:  0.37500E+34 -0.48000E+01  0.19000E+04
     TROE centering:      0.64640E+00  0.13200E+03  0.13150E+04  0.55660E+04
        H2               Enhanced by    2.000E+00
        H2O              Enhanced by    6.000E+00
        CH4              Enhanced by    2.000E+00
        CO               Enhanced by    1.500E+00
        CO2              Enhanced by    2.000E+00
        C2H6             Enhanced by    3.000E+00
246. H+C2H2(+M)<=>C2H3(+M)                       5.600E+12    0.00    2400.0
     Low pressure limit:  0.38000E+41 -0.72700E+01  0.72200E+04
     TROE centering:      0.75070E+00  0.98500E+02  0.13020E+04  0.41670E+04
        H2               Enhanced by    2.000E+00
        H2O              Enhanced by    6.000E+00
        CH4              Enhanced by    2.000E+00
        CO               Enhanced by    1.500E+00
        CO2              Enhanced by    2.000E+00
        C2H6             Enhanced by    3.000E+00
247. H+C2H3(+M)<=>C2H4(+M)                       6.080E+12    0.27     280.0
     Low pressure limit:  0.14000E+31 -0.38600E+01  0.33200E+04
     TROE centering:      0.78200E+00  0.20750E+03  0.26630E+04  0.60950E+04
        H2               Enhanced by    2.000E+00
        H2O              Enhanced by    6.000E+00
        CH4              Enhanced by    2.000E+00
        CO               Enhanced by    1.500E+00
        CO2              Enhanced by    2.000E+00
        C2H6             Enhanced by    3.000E+00
248. H+C2H3<=>H2+C2H2                            3.000E+13    0.00       0.0
249. H+C2H4(+M)<=>C2H5(+M)                       5.400E+11    0.45    1820.0
     Low pressure limit:  0.60000E+42 -0.76200E+01  0.69700E+04
     TROE centering:      0.97530E+00  0.21000E+03  0.98400E+03  0.43740E+04
        H2               Enhanced by    2.000E+00
        H2O              Enhanced by    6.000E+00
        CH4              Enhanced by    2.000E+00
        CO               Enhanced by    1.500E+00
        CO2              Enhanced by    2.000E+00
        C2H6             Enhanced by    3.000E+00
250. H+C2H4<=>C2H3+H2                            1.325E+06    2.53   12240.0
251. H+C2H5(+M)<=>C2H6(+M)                       5.210E+17   -0.99    1580.0
     Low pressure limit:  0.19900E+42 -0.70800E+01  0.66850E+04
     TROE centering:      0.84220E+00  0.12500E+03  0.22190E+04  0.68820E+04
        H2               Enhanced by    2.000E+00
        H2O              Enhanced by    6.000E+00
        CH4              Enhanced by    2.000E+00
        CO               Enhanced by    1.500E+00
        CO2              Enhanced by    2.000E+00
        C2H6             Enhanced by    3.000E+00
252. H+C2H5<=>H2+C2H4                            2.000E+12    0.00       0.0
253. H+C2H6<=>C2H5+H2                            1.150E+08    1.90    7530.0
254. H+HCCO<=>CH2(S)+CO                          1.000E+14    0.00       0.0
255. H+HCCOH<=>H+CH2CO                           1.000E+13    0.00       0.0
256. H2+CO(+M)<=>CH2O(+M)                        4.300E+07    1.50   79600.0
     Low pressure limit:  0.50700E+28 -0.34200E+01  0.84350E+05
     TROE centering:      0.93200E+00  0.19700E+03  0.15400E+04  0.10300E+05
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        H2               Enhanced by    2.000E+00
        H2O              Enhanced by    6.000E+00
        CH4              Enhanced by    2.000E+00
        CO               Enhanced by    1.500E+00
        CO2              Enhanced by    2.000E+00
        C2H6             Enhanced by    3.000E+00
257. 2OH(+M)<=>H2O2(+M)                        7.400E+13   -0.37       0.0
     Low pressure limit:  0.23000E+19 -0.90000E+00 -0.17000E+04
     TROE centering:      0.73460E+00  0.94000E+02  0.17560E+04  0.51820E+04
        H2               Enhanced by    2.000E+00
        H2O              Enhanced by    6.000E+00
        CH4              Enhanced by    2.000E+00
        CO               Enhanced by    1.500E+00
        CO2              Enhanced by    2.000E+00
        C2H6             Enhanced by    3.000E+00
258. OH+CH2<=>H+CH2O                           2.000E+13    0.00       0.0
259. OH+CH2<=>CH+H2O                           1.130E+07    2.00    3000.0
260. OH+CH2(S)<=>H+CH2O                        3.000E+13    0.00       0.0
261. OH+CH3(+M)<=>CH3OH(+M)                    2.790E+18   -1.43    1330.0
     Low pressure limit:  0.40000E+37 -0.59200E+01  0.31400E+04
     TROE centering:      0.41200E+00  0.19500E+03  0.59000E+04  0.63940E+04
        H2               Enhanced by    2.000E+00
        H2O              Enhanced by    6.000E+00
        CH4              Enhanced by    2.000E+00
        CO               Enhanced by    1.500E+00
        CO2              Enhanced by    2.000E+00
        C2H6             Enhanced by    3.000E+00
262. OH+CH3<=>CH2+H2O                          5.600E+07    1.60    5420.0
263. OH+CH3<=>CH2(S)+H2O                       6.440E+17   -1.34    1417.0
264. OH+CH4<=>CH3+H2O                          1.000E+08    1.60    3120.0
265. OH+CH2O<=>HCO+H2O                         3.430E+09    1.18    -447.0
266. OH+CH2OH<=>H2O+CH2O                       5.000E+12    0.00       0.0
267. OH+CH3O<=>H2O+CH2O                        5.000E+12    0.00       0.0
268. OH+CH3OH<=>CH2OH+H2O                      1.440E+06    2.00    -840.0
269. OH+CH3OH<=>CH3O+H2O                       6.300E+06    2.00    1500.0
270. OH+C2H<=>H+HCCO                           2.000E+13    0.00       0.0
271. OH+C2H2<=>H+CH2CO                         2.180E-04    4.50   -1000.0
272. OH+C2H2<=>H+HCCOH                         5.040E+05    2.30   13500.0
273. OH+C2H2<=>C2H+H2O                         3.370E+07    2.00   14000.0
274. OH+C2H2<=>CH3+CO                          4.830E-04    4.00   -2000.0
275. OH+C2H3<=>H2O+C2H2                        5.000E+12    0.00       0.0
276. OH+C2H4<=>C2H3+H2O                        3.600E+06    2.00    2500.0
277. OH+C2H6<=>C2H5+H2O                        3.540E+06    2.12     870.0
278. OH+CH2CO<=>HCCO+H2O                       7.500E+12    0.00    2000.0
279. HO2+CH2<=>OH+CH2O                         2.000E+13    0.00       0.0
280. HO2+CH3<=>O2+CH4                          1.000E+12    0.00       0.0
281. HO2+CH3<=>OH+CH3O                         2.000E+13    0.00       0.0
282. HO2+CH2O<=>HCO+H2O2                       5.600E+06    2.00   12000.0
283. C+CH2<=>H+C2H                             5.000E+13    0.00       0.0
284. C+CH3<=>H+C2H2                            5.000E+13    0.00       0.0
285. CH+H2<=>H+CH2                             1.080E+14    0.00    3110.0
286. CH+H2O<=>H+CH2O                           5.710E+12    0.00    -755.0
287. CH+CH2<=>H+C2H2                           4.000E+13    0.00       0.0
288. CH+CH3<=>H+C2H3                           3.000E+13    0.00       0.0
289. CH+CH4<=>H+C2H4                           6.000E+13    0.00       0.0
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290. CH+CO(+M)<=>HCCO(+M)                          5.000E+13    0.00       0.0
     Low pressure limit:  0.26900E+29 -0.37400E+01  0.19360E+04
     TROE centering:      0.57570E+00  0.23700E+03  0.16520E+04  0.50690E+04
        H2               Enhanced by    2.000E+00
        H2O              Enhanced by    6.000E+00
        CH4              Enhanced by    2.000E+00
        CO               Enhanced by    1.500E+00
        CO2              Enhanced by    2.000E+00
        C2H6             Enhanced by    3.000E+00
291. CH+CH2O<=>H+CH2CO                             9.460E+13    0.00    -515.0
292. CH+HCCO<=>CO+C2H2                             5.000E+13    0.00       0.0
293. CH2+O2=>OH+H+CO                               5.000E+12    0.00    1500.0
294. CH2+H2<=>H+CH3                                5.000E+05    2.00    7230.0
295. 2CH2<=>H2+C2H2                                1.600E+15    0.00   11944.0
296. CH2+CH3<=>H+C2H4                              4.000E+13    0.00       0.0
297. CH2+CH4<=>2CH3                                2.460E+06    2.00    8270.0
298. CH2+HCCO<=>C2H3+CO                            3.000E+13    0.00       0.0
299. CH2(S)+N2<=>CH2+N2                            1.500E+13    0.00     600.0
300. CH2(S)+O2<=>H+OH+CO                           2.800E+13    0.00       0.0
301. CH2(S)+O2<=>CO+H2O                            1.200E+13    0.00       0.0
302. CH2(S)+H2<=>CH3+H                             7.000E+13    0.00       0.0
303. CH2(S)+H2O(+M)<=>CH3OH(+M)                    4.820E+17   -1.16    1145.0
     Low pressure limit:  0.18800E+39 -0.63600E+01  0.50400E+04
     TROE centering:      0.60270E+00  0.20800E+03  0.39220E+04  0.10180E+05
        H2               Enhanced by    2.000E+00
        H2O              Enhanced by    6.000E+00
        CH4              Enhanced by    2.000E+00
        CO               Enhanced by    1.500E+00
        CO2              Enhanced by    2.000E+00
        C2H6             Enhanced by    3.000E+00
304. CH2(S)+H2O<=>CH2+H2O                          3.000E+13    0.00       0.0
305. CH2(S)+CH3<=>H+C2H4                           1.200E+13    0.00    -570.0
306. CH2(S)+CH4<=>2CH3                             1.600E+13    0.00    -570.0
307. CH2(S)+CO<=>CH2+CO                            9.000E+12    0.00       0.0
308. CH2(S)+CO2<=>CH2+CO2                          7.000E+12    0.00       0.0
309. CH2(S)+CO2<=>CO+CH2O                          1.400E+13    0.00       0.0
310. CH2(S)+C2H6<=>CH3+C2H5                        4.000E+13    0.00    -550.0
311. CH3+O2<=>O+CH3O                               3.560E+13    0.00   30480.0
312. CH3+O2<=>OH+CH2O                              2.310E+12    0.00   20315.0
313. CH3+H2O2<=>HO2+CH4                            2.450E+04    2.47    5180.0
314. 2CH3(+M)<=>C2H6(+M)                           6.770E+16   -1.18     654.0
     Low pressure limit:  0.34000E+42 -0.70300E+01  0.27620E+04
     TROE centering:      0.61900E+00  0.73200E+02  0.11800E+04  0.99990E+04
        H2               Enhanced by    2.000E+00
        H2O              Enhanced by    6.000E+00
        CH4              Enhanced by    2.000E+00
        CO               Enhanced by    1.500E+00
        CO2              Enhanced by    2.000E+00
        C2H6             Enhanced by    3.000E+00
315. 2CH3<=>H+C2H5                                 6.840E+12    0.10   10600.0
316. CH3+HCO<=>CH4+CO                              2.648E+13    0.00       0.0
317. CH3+CH2O<=>HCO+CH4                            3.320E+03    2.81    5860.0
318. CH3+CH3OH<=>CH2OH+CH4                         3.000E+07    1.50    9940.0
319. CH3+CH3OH<=>CH3O+CH4                          1.000E+07    1.50    9940.0
320. CH3+C2H4<=>C2H3+CH4                           2.270E+05    2.00    9200.0
321. CH3+C2H6<=>C2H5+CH4                           6.140E+06    1.74   10450.0
322. CH2OH+O2<=>HO2+CH2O                           1.800E+13    0.00     900.0
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323. CH3O+O2<=>HO2+CH2O                          4.280E-13    7.60   -3530.0
324. C2H+O2<=>HCO+CO                             1.000E+13    0.00    -755.0
325. C2H+H2<=>H+C2H2                             5.680E+10    0.90    1993.0
326. C2H3+O2<=>HCO+CH2O                          4.580E+16   -1.39    1015.0
327. C2H4(+M)<=>H2+C2H2(+M)                      8.000E+12    0.44   86770.0
     Low pressure limit:  0.15800E+52 -0.93000E+01  0.97800E+05
     TROE centering:      0.73450E+00  0.18000E+03  0.10350E+04  0.54170E+04
        H2               Enhanced by    2.000E+00
        H2O              Enhanced by    6.000E+00
        CH4              Enhanced by    2.000E+00
        CO               Enhanced by    1.500E+00
        CO2              Enhanced by    2.000E+00
        C2H6             Enhanced by    3.000E+00
328. C2H5+O2<=>HO2+C2H4                          8.400E+11    0.00    3875.0
329. 2HCCO<=>2CO+C2H2                            1.000E+13    0.00       0.0
330. NNH+CH3<=>CH4+N2                            2.500E+13    0.00       0.0
331. NNH+O2<=>HO2+N2                             5.000E+12    0.00       0.0
332. NNH+O<=>OH+N2                               2.500E+13    0.00       0.0
333. H2CN+N<=>N2+CH2                             6.000E+13    0.00     400.0
334. CH2+N2<=>HCN+NH                             1.000E+13    0.00   74000.0
335. CH2(S)+N2<=>NH+HCN                          1.000E+11    0.00   65000.0
336. C+NO<=>CO+N                                 2.900E+13    0.00       0.0
337. CH+NO<=>H+NCO                               1.620E+13    0.00       0.0
338. CH+NO<=>N+HCO                               2.460E+13    0.00       0.0
339. CH2+NO<=>H+HNCO                             3.100E+17   -1.38    1270.0
340. CH2+NO<=>OH+HCN                             2.900E+14   -0.69     760.0
341. CH2+NO<=>H+HCNO                             3.800E+13   -0.36     580.0
342. CH2(S)+NO<=>H+HNCO                          3.100E+17   -1.38    1270.0
343. CH2(S)+NO<=>OH+HCN                          2.900E+14   -0.69     760.0
344. CH2(S)+NO<=>H+HCNO                          3.800E+13   -0.36     580.0
345. CH3+NO<=>HCN+H2O                            9.600E+13    0.00   28800.0
346. CH3+NO<=>H2CN+OH                            1.000E+12    0.00   21750.0
347. HCNO+H<=>H+HNCO                             2.100E+15   -0.69    2850.0
348. HCNO+H<=>OH+HCN                             2.700E+11    0.18    2120.0
349. HCNO+H<=>NH2+CO                             1.700E+14   -0.75    2890.0
350. CH3+N<=>H2CN+H                              6.100E+14   -0.31     290.0
351. CH3+N<=>HCN+H2                              3.700E+12    0.15     -90.0
352. OH+NO2(+M)=HNO3(+M)                         2.410E+13    0.00       0.0
     Low pressure limit:  0.64200E+33 -0.54900E+01  0.23500E+04
     T&H VALUES  0.72500E+00 -0.25000E-03
        N2O              Enhanced by    5.000E+00
        H2O              Enhanced by    9.000E+00
        N2               Enhanced by    1.000E+00
        HNO3             Enhanced by    5.000E+00
        NH3              Enhanced by    5.000E+00
        NO3              Enhanced by    5.000E+00
353. HNO3+H=NO3+H2                               2.400E+08    1.50   11600.0
354. HNO3+H=NO2+H2O                              6.000E+13    0.00    9800.0
355. HNO3+H=HNO2+OH                              6.000E+13    0.00    7000.0
356. HNO3+H=HONO+OH                              2.000E+13    0.00    8000.0
357. HNO3+O=NO3+OH                               2.000E+13    0.00   12000.0
358. HNO3+OH=H2O+NO3                             4.340E+09    0.00   -1560.0
359. HNO3+OH(+M)=H2O+NO3(+M)                     2.470E+08    0.00   -2860.0
     Low pressure limit:  0.68900E+15  0.00000E+00 -0.14400E+04
        N2O              Enhanced by    5.000E+00
        H2O              Enhanced by    9.000E+00
        N2               Enhanced by    1.000E+00
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        HNO3             Enhanced by    5.000E+00
        NH3              Enhanced by    5.000E+00
        NO3              Enhanced by    5.000E+00
360. NO3+H2O2=HNO3+HO2                           1.000E+12    0.00    8500.0

361. HNO3+NH=HNOH+NO2                            1.500E+13    0.00    6000.0
362. HNO3+NH2=NO3+NH3                            9.000E+05    2.00    7300.0
363. HNO3+NH2=NH2O+HNO2                          3.000E+12    0.00    9000.0
364. HNO3+NH3=NH2O+H2O+NO                        2.320E+01    3.50   44930.0
365. HNO3+NO=HONO+NO2                            8.000E+06    2.00   11000.0
366. HONO+NO3=HNO3+NO2                           1.000E+12    0.00    6000.0
367. HNO2+NO3=HNO3+NO2                           1.000E+12    0.00    5000.0
368. O+NO2(+M)=NO3(+M)                           1.330E+13    0.00       0.0
     Low pressure limit:  0.14900E+29 -0.40800E+01  0.24700E+04
     T&H VALUES  0.79000E+00 -0.18000E-03
        N2O              Enhanced by    5.000E+00
        H2O              Enhanced by    9.000E+00
        N2               Enhanced by    1.000E+00
        HNO3             Enhanced by    5.000E+00
        NH3              Enhanced by    5.000E+00
        NO3              Enhanced by    5.000E+00
369. NO3+H=NO2+OH                                6.000E+13    0.00       0.0
370. NO3+O=NO2+O2                                1.000E+13    0.00       0.0
371. NO3+OH=HO2+NO2                              1.200E+13    0.00       0.0
372. NO3+HO2=NO2+O2+OH                           2.500E+12    0.00       0.0
373. NO3+NH=HNO+NO2                              1.500E+13    0.00       0.0
374. NO3+NH=HNO3+N                               1.000E+12    0.00    5000.0
375. NO3+NH2=HNO3+NH                             1.000E+12    0.00   10000.0
376. NO3+NH2=NH2O+NO2                            9.000E+05    0.00     100.0
377. NO3+NO3=2NO2+O2                             5.120E+11    0.00    4870.0
378. NO2+HO2=HONO+O2                             1.000E+12    0.00    5000.0
379. HNOH+NO2=HONO+HNO                           6.000E+11    0.00    2000.0
380. HNOH+H=NH2+OH                               4.000E+13    0.00       0.0
381. HNOH+H=HNO+H2                               4.800E+08    1.50     378.0
382. HNOH+O=HNO+OH                               7.000E+13    0.00       0.0
     Declared duplicate reaction...
383. HNOH+O=HNO+OH                               3.300E+08    1.50    -358.0
     Declared duplicate reaction...
384. HNOH+OH=HNO+H2O                             2.400E+06    2.00   -1192.0
385. NH2O+H=NH2+OH                               4.000E+13    0.00       0.0
386. NH2O+H=HNO+H2                               4.800E+08    1.50    1560.0
387. NH2O+O=HNO+OH                               3.300E+08    1.50     487.0
388. NH2O+OH=HNO+H2O                             2.400E+06    2.00   -1192.0
389. NH2O+NH2=HNO+NH3                            1.800E+06    1.94   -1152.0
390. HNO2+H=H2+NO2                               2.400E+08    1.50    4163.0
391. HNO2+O=OH+NO2                               1.700E+08    1.50    2365.0
392. HNO2+OH=H2O+NO2                             1.200E+06    2.00    -795.0
393. HNO2+NH2=NO2+NH3                            9.200E+05    1.94     874.0
394. NO3+CH2O=HNO3+HCO                           1.700E+12    0.00    5000.0
395. NO3+HCO=H+CO2+NO2                           2.000E+13    0.00       0.0
396. NO3+C2H4=C2H4O+NO2                          2.000E+12    0.00    5720.0
397. C2H4O=CH4+CO                                1.210E+13    0.00   57200.0
398. C2H4O=CH3CHO                                7.260E+13    0.00   57200.0
399. C2H4O=CH3+HCO                               3.630E+13    0.00   57200.0
400. C2H4O+CH3=CH4+CH2CHO                        1.100E+12    0.00   11800.0
401. C2H4O+OH=H2O+CH2CHO                         1.400E+13    0.00    3360.0
402. C2H4O+H=H2+CH2CHO                           3.800E+13    0.00    9197.0
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403. C2H4O+NO2=HONO+CH2CHO                          1.300E+12    0.00    3700.0
404. C2H4O+NO3=HNO3+CH2CHO                          1.000E+12    0.00    6000.0
405. CH2CHO+H=CH3+HCO                               1.000E+14    0.00       0.0
406. CH2CHO+H=H2+CH2CO                              1.000E+13    0.00       0.0
407. CH2CHO+OH=CH2OH+HCO                            2.000E+13    0.00       0.0
408. CH2CHO+OH=CH2CO+H2O                            1.200E+06    2.00       0.0
409. CH2CHO+NO=HNO+CH2CO                            1.000E+12    0.00    8600.0
410. CH2CHO+NO2=HONO+CH2CO                          8.900E+12    0.00    -160.0
411. CH2CHO+NO3=HNO3+CH2CO                          1.000E+12    0.00       0.0
412. CH3+NO3=CH3O+NO2                               2.000E+13    0.00       0.0
413. O+C2H5<=>H+CH3CHO                              1.096E+14    0.00       0.0
414. O+CH3CHO<=>OH+CH2CHO                           2.920E+12    0.00    1808.0
415. O+CH3CHO=>OH+CH3+CO                            2.920E+12    0.00    1808.0
416. O2+CH3CHO=>HO2+CH3+CO                          3.010E+13    0.00   39150.0
417. H+CH3CHO<=>CH2CHO+H2                           2.050E+09    1.16    2405.0
418. H+CH3CHO=>CH3+H2+CO                            2.050E+09    1.16    2405.0
419. OH+CH3CHO=>CH3+H2O+CO                          2.343E+10    0.73   -1113.0
420. HO2+CH3CHO=>CH3+H2O2+CO                        3.010E+12    0.00   11923.0
421. CH3+CH3CHO=>CH3+CH4+CO                         2.720E+06    1.77    5920.0
422. O+C2H4<=>H+CH2CHO                              6.700E+06    1.83     220.0
423. C2H3+O2<=>O+CH2CHO                             3.030E+11    0.29      11.0
424. C2H3+O2<=>HO2+C2H2                             1.337E+06    1.61    -384.0
425. H+CH2CO(+M)<=>CH2CHO(+M)                       4.865E+11    0.42   -1755.0
      Low pressure limit:  0.10120E+43 -0.76300E+01  0.38540E+04
      TROE centering:      0.46500E+00  0.20100E+03  0.17730E+04  0.53330E+04
         H2               Enhanced by    2.000E+00
         H2O              Enhanced by    6.000E+00
         CO               Enhanced by    1.500E+00
         CO2              Enhanced by    2.000E+00
426. O+CH2CHO=>H+CH2+CO2                            1.500E+14    0.00       0.0
427. O2+CH2CHO=>OH+CO+CH2O                          1.810E+10    0.00       0.0
428. CH3+NH=H2CN+H2                                 3.500E+13    0.00     290.0
429. HCO+HNO=CH2O+NO                                6.000E+11    0.00    2000.0
430. CH2O+NO2=HCO+HONO                              8.020E+02    2.77   13730.0
431. HCO+NO2=CO+HONO                                1.240E+23   -3.29    2355.0
432. HCO+NO2=H+CO2+NO                               8.390E+15   -0.75    1930.0
433. HCO+HCO=CH2O+CO                                3.000E+13    0.00       0.0
434. HCO+HCO=H2+CO+CO                               5.200E+12    0.00       0.0
435. CH4+NO2=CH3+HONO                               1.200E+13    0.00   30000.0
436. CH3+NO2=CH3O+NO                                1.400E+13    0.00       0.0
437. CH2+NO2=CH2O+NO                                5.000E+13    0.00       0.0
438. H2CN+N=HCN+NH                                  7.200E+13    0.00     400.0
439. H2CN+H=HCN+H2                                  4.000E+13    0.00       0.0
440. OH+HCN=HOCN+H                                  1.100E+06    2.03   13373.0
441. HOCN+H=HNCO+H                                  3.100E+08    0.84    1917.0
442. HOCN+H=NH2+CO                                  1.200E+08    0.61    2076.0
443. HOCN+H=H2+NCO                                  2.400E+08    1.50    6617.0
444. CH3NHNH2+M=CH3NH+NH2+M                         2.500E+14    0.00   40940.0
445. CH3NHNH2+H=CH3NNH2+H2                          1.300E+13    0.00    2500.0
446. CH3NHNH2+H=CH3NH+NH3                           4.460E+09    0.00    3100.0
447. CH3NHNH2+CH3=CH4+CH3NNH2                       1.000E+13    0.00    6990.0
448. CH3NHNH2+NH2=NH3+CH3NNH2                       1.000E+11    0.50    1990.0
449. CH3NNH2+M=CH3NNH+H+M                           1.000E+17    0.00   35770.0
450. CH3NH+M=CH3+NH+M                               1.000E+14    0.00   18000.0
451. CH3NH+M=CH2NH+H+M                              1.000E+16    0.00   23800.0
452. CH3NH+H=CH2NH+H2                               1.000E+08    2.00       0.0
453. CH3NH+H=CH3+NH2                                6.000E+13    0.00       0.0
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454. CH3NNH+CH3=CH4+CH3NN                          4.600E+13    0.00    4850.0
455. CH3NNH+NH2=NH3+CH3NN                          4.600E+13    0.00    4850.0
456. CH3NN=CH3+N2                                  3.000E+06    0.00       0.0
457. CH3NNCH3=CH3NN+CH3                            6.900E+15    0.00   50880.0
458. CH3NNCH3=C2H6+N2                              2.000E+11    0.00   33000.0
459. CH2NH+M=HCN+H2+M                              1.000E+14    0.00   10000.0
460. CH3NHNH2=CH3NNH+H2                            3.160E+13    0.00   57000.0
461. CH3NHNH2=CH2NH+NH3                            1.580E+13    0.00   54000.0
462. CH3NNH2+HO2=CH3NHNH2+O2                       1.000E+06    2.00       0.0
463. CH3NN+HO2=CH3NNH+O2                           1.000E+06    2.00       0.0
464. CH3NHNH2+O=CH3NNH+H2O                         9.600E+12    0.00       0.0
465. CH3NNH2+OH=CH3NNH+H2O                         1.000E+08    2.00       0.0
466. CH3NNH2+O=CH3NNH+OH                           1.000E+08    2.00       0.0
467. CH3NNH2+HO2=CH3NNH+H2O2                       1.000E+08    2.00       0.0
468. CH3NNH2+O2=CH3NNH+HO2                         4.000E+12    0.00       0.0
469. CH3NHNH2+HO2=CH3NNH2+H2O2                     2.700E+11    0.00    1987.0
470. CH3NNH+HO2=CH3NN+H2O2                         1.000E+11    0.00    1987.0
471. CH3NHNH2+OH=CH3NNH2+H2O                       3.920E+13    0.00       0.0
472. CH3NNH+OH=CH3NN+H2O                           3.920E+13    0.00       0.0
473. CH3NHNH2+O=CH3NNH2+OH                         9.600E+12    0.00       0.0
474. CH3NNH+O=CH3NN+OH                             9.600E+12    0.00       0.0
475. CH3NH+OH=CH2NH+H2O                            1.000E+08    2.00       0.0
476. CH3NH+O=CH2NH+OH                              1.000E+08    2.00       0.0
477. CH3NH+O2=CH2NH+HO2                            1.000E+07    2.00    6300.0
478. CH3NH+O=CH3O+NH                               6.000E+13    0.00       0.0
479. CH3NH+OH=CH4+HNO                              6.000E+12    0.00       0.0
480. CH3NH+O2=CH3O+HNO                             6.000E+12    0.00    4000.0
481. CH2NH+O=CH2O+NH                               1.000E+07    2.00    2800.0
482. CH2NH+OH=CH2O+NH2                             1.800E+05    2.00   14800.0
483. CH2NH+O=H2CN+OH                               3.160E+08    2.00    6100.0
484. H2CN+HO2=CH2NH+O2                             7.870E+04    2.00   21700.0
485. CH2NH+OH=H2CN+H2O                             1.000E+07    2.00    4000.0
486. H2CN+O=HCN+OH                                 1.000E+07    2.00    6100.0
487. H2CN+OH=HCN+H2O                               1.000E+07    2.00    3700.0
488. H2CN+O2=HCN+HO2                               2.700E+04    2.00   17300.0
489. H2CN+NO=HCN+HNO                               1.000E+07    2.00    4400.0
490. CH3NNH2+NO2(+M)=CH3N(NH2)NO2(+M)              1.000E+13    0.00       0.0
     Low pressure limit:  0.10000E+18  0.00000E+00  0.00000E+00
491. CH3NNH2+NO2(+M)=CH3N(NH2)ONO(+M)              1.000E+13    0.00       0.0
     Low pressure limit:  0.10000E+18  0.00000E+00  0.00000E+00
492. CH3NHNH2+NO2=CH3NNH2+HONO                     2.200E+11    0.00    5900.0
493. CH3NNH+NO2=CH3NN+HONO                         2.200E+11    0.00    5900.0
494. CH3NNH2+NO2=CH3NNH+HONO                       1.000E+08    2.00       0.0
495. NH2+HO2=NH3+O2                                2.000E+13    0.00       0.0
496. N2O4(+M)=NO2+NO2(+M)                          4.050E+18   -1.10   12840.0
     Low pressure limit:  0.19600E+29 -0.38000E+01  0.12800E+05
497. CH3NHNH2+HNO3=NAMMH                           2.000E+13    0.00       0.0
498. CH3NO2(+M)=CH3+NO2(+M)                        1.800E+16    0.00   58500.0
     Low pressure limit:  0.13000E+18  0.00000E+00  0.42000E+05
     T&H VALUE  0.18300E+00
499. CH3NO2+H=CH3+HONO                             3.300E+12    0.00    3730.0
500. CH3NO2+H=CH3NO+OH                             1.400E+12    0.00    3730.0
501. CH3NO2+H=H2CNO2+H2                            5.400E+02    3.50    5200.0
502. CH3NO2+O=H2CNO2+OH                            1.500E+13    0.00    5350.0
503. CH3NO2+OH=H2CNO2+H2O                          5.000E+05    2.00    1000.0
504. CH3NO2+OH=CH3OH+NO2                           2.000E+10    0.00   -1000.0
505. CH3NO2+CH3=H2CNO2+CH4                         5.500E-01    4.00    8300.0
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506. CH3NO2+CH2(S)=H2CNO2+CH3                    1.200E+14    0.00       0.0
507. CH3NO2+CH2=H2CNO2+CH3                       6.500E+12    0.00    7900.0
508. H2CNO2=CH2O+NO                              1.000E+13    0.00   36000.0
509. CH3+NO(+M)=CH3NO(+M)                        9.000E+12    0.00     119.0
     Low pressure limit:  0.32000E+24 -0.18700E+01  0.00000E+00
510. CH3O+NO=CH2O+HNO                            1.300E+14   -0.70       0.0
511. CH3O+NO(+M)=CH3ONO(+M)                      6.600E+14   -0.60       0.0
     Low pressure limit:  0.27000E+28 -0.35000E+01  0.00000E+00
512. CH3O+NO2=CH2O+HONO                          6.000E+12    0.00    2285.0
513. CH3O+NO2(+M)=CH3ONO2(+M)                    1.200E+13    0.00       0.0
     Low pressure limit:  0.14000E+31 -0.45000E+01  0.00000E+00
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